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October 28, 2015

APS March Meeting
Baltimore, MD, United States
March 14, 2016 through March 18, 2016

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High-pressure X-ray diffraction, Raman, and computational studies of MgCl_2 up to 1 Mbar: Extensive pressure stability of the $\beta\text{-MgCl}_2$ layered structure.

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Magnesium chloride with the rhombohedral layered CdCl_2 -type structure ($\alpha\text{-MgCl}_2$) has been studied using x-ray diffraction and Raman spectroscopy up to 1 Mbar (at RT). The results reveal a pressure-induced second-order phase transition to a hexagonal layered CdI_2 -type structure ($\beta\text{-MgCl}_2$) at 0.7 GPa. This phase transition mainly affects the stacking sequence of the Cl anions, resulting to a shorter c -axis. An anisotropic compression along the c -axis was observed during initial compression. Above 10 GPa, the anisotropy is altered due to the repulsion of Cl anions between adjacent perpendicular to c -axis Cl-layers.

According to previous theoretical studies, a series of phase transitions towards, initially, the 3D rutile structure (with 6-fold coordinated Mg cations) at ~ 17 GPa and to fluorite structure (with 8-fold coordinated Mg cations) at ~ 70 GPa are proposed. However, according to our experimental results MgCl_2 remains in a 2D layered structure up to 1Mbar keeping the 6-fold coordination of Mg cations. This observation contradicts with the general structural behavior of highly compressed AB_2 compounds; we conducted *ab-initio* DFT theoretical calculations to elucidate the mechanisms that extend the remarkable structural stability of MgCl_2 .

This work was performed under the auspices of the U. S. Department of Energy by Lawrence Livermore National Security, LLC under Contract DE-AC52-07NA27344.